

3,4-Hexanediol, 3,4-dimethyl-

Inchi:	InChI=1S/C8H18O2/c1-5-7(3,9)8(4,10)6-2/h9-10H,5-6H2,1-4H3
InchiKey:	RJOVKNVJGPMWDT-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CCC(C)(O)C(C)(O)CC
Mol. weight [g/mol]:	146.23
CAS:	1185-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-251.48	kJ/mol	Joback Method
hf	-530.41	kJ/mol	Joback Method
hfus	9.82	kJ/mol	Joback Method
hvap	64.17	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.308		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	560.34	K	Joback Method
tc	732.08	K	Joback Method
tf	326.00 ± 3.00	K	NIST Webbook
vc	0.499	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.75	J/mol×K	560.34	Joback Method
cpg	362.94	J/mol×K	588.96	Joback Method
cpg	373.51	J/mol×K	617.59	Joback Method
cpg	383.50	J/mol×K	646.21	Joback Method
cpg	392.93	J/mol×K	674.83	Joback Method
cpg	401.85	J/mol×K	703.45	Joback Method
cpg	410.29	J/mol×K	732.08	Joback Method
dvisc	0.0655747	Paxs	306.40	Joback Method
dvisc	0.0091067	Paxs	348.72	Joback Method

dvisc	0.0019390	Paxs	391.05	Joback Method
dvisc	0.0005585	Paxs	433.37	Joback Method
dvisc	0.0002007	Paxs	475.69	Joback Method
dvisc	0.0000853	Paxs	518.02	Joback Method
dvisc	0.0000412	Paxs	560.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1185020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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